Manifestations of hyperfine interaction in plasticity

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A mechanism is proposed of how the hyperfine interaction of the electron and nuclear spins in the paramagnetic obstacle–dislocation system may influence the plastic properties of crystals in a magnetic field. It is shown that the hyperfine interaction leads to a threshold-type behavior of the magnetic-field dependence of various plasticity-related quantities. A strong influence of the hyperfine interaction on the behavior of the internal friction of dislocations in weak magnetic fields is predicted. [S0163-1829(97)01142-9]

The theory of mechanical properties of crystals usually considers nuclei as point charges disregarding their internal structure. A similar approximation has been widely used in the theory of electronic structure of molecules. This approximation is justified as long as various characteristics of nuclei, such as mass, spin, size, and shape, do not appreciably influence static properties of molecules or crystals. However, it is known that the role of nuclear magnetic moments may appear to be of importance for chemical reaction rates in a magnetic field.[1,2] This leads to the phenomenon called the magnetic isotope effect in chemical reactions in which the hyperfine interaction of the electron and nuclear spins changes populations of various electronic states of radical pairs thereby changing their chemical reactivity.

When addressing plasticity-related phenomena we have to consider the motion of dislocations and their pinning by point defects—obstacles. The dynamics of formation of the obstacle–dislocation bonds in a magnetic field was recently discussed in Ref. 3 (see also Refs. 4–7 discussing various plasticity-related phenomena). It is assumed that the dangling bond of a paramagnetic obstacle forms a radical pair with a dangling bond of the dislocation core. The magnetic field influences the transitions between different spin states of such pairs, which are characterized by different binding energies, and thus changes the depinning probability. This is a mechanism of how the plastic properties of crystals (both metals and dielectrics) may be influenced by a magnetic field in a broad temperature range. In pure undeformed metals at low temperatures there is also a large contribution from the Kravchenko mechanism,[8] in which the magnetic field increases the electron component of the dislocation viscous drag.

An analogy with chemical reaction theory suggests that a hyperfine interaction in the obstacle–dislocation system also may play an important role in plasticity of crystals in a magnetic field. This may also lead to a magnetic isotope effect in plasticity. This paper discusses the part played by the hyperfine interaction in the dynamics of obstacle–dislocation radical pairs in a magnetic field and presents results for several experimentally measurable quantities.

The influence of hyperfine interactions on the plasticity will be considered within the framework of the model outlined in Ref. 3, which considers the dislocation motion at low stresses, not exceeding the Peierls stress, which occurs by means of depinning of dislocation kinks from paramagnetic obstacles. Unsaturated electron states in the kink and the obstacle form a radical pair whose binding energy depends strongly on the total spin of the pair. This energy is usually much higher in the singlet S state than in a triplet T state. The pair in a T state allows the kink to pass the obstacle freely and the dislocation depins. This model allows one to explain various effects related to a change of plasticity in a magnetic field.[3]

Now we modify this model by introducing an interaction between the spins of electrons forming the radical pair and the spins of nuclei of the obstacle or/and dislocation core. The simple, but still rather general, situation is considered here when only one nucleus in the kink-obstacle radical pair has a nonzero spin $I=1/2$. Then the spin Hamiltonian of the system can be written in the form

$$\mathcal{H}=g_1\mu_B\mathbf{H}\cdot\hat{\mathbf{S}}_1+g_2\mu_B\mathbf{H}\cdot\hat{\mathbf{S}}_2+A\mathbf{S}_1\cdot\hat{\mathbf{I}}_1, \tag{1}$$

where g_1 and g_2 are g factors of the kink and obstacle electron states forming the radical pair, μ_B is the Bohr magneton, $\mathbf{H}$ is the magnetic-field vector. $\hat{\mathbf{S}}_1$ and $\hat{\mathbf{S}}_2$ are the corresponding spin operators. $\hat{\mathbf{I}}_1$ is the nuclear-spin operator which is chosen to relate to one of the nuclei in the radical pair. Generalization to other possible nuclear-spin configurations is straightforward.

The hyperfine interaction couples the S state of the radical pair with all three of its triplet states, T_0, T_+, and T_-. Typical values of the hyperfine coupling constant A varies from 1 to 100 Oe. The $S-T_\pm$ transitions are of importance only in a low magnetic field, $H<A$, when the degenerate triplet may be in a resonance with the S state. At higher magnetic fields, $H>A$, the Zeeman splitting lifts the degeneracy of the triplet so that only the T_0 state remains in resonance with the S state and only the $S-T_0$ transitions are then of importance. The condition $H>A$ will be assumed in what follows.

Nuclear spins are characterized by very large relaxation times in a rather broad temperature range. Even in metals the characteristic values of the relaxation times lie in the range from 10^{-3} to 10^{-2} s at room temperature.[9] They are much longer in dielectrics. This time scale should be compared with the characteristic time during which a kink may pass an obstacle, 10^{-7} s.[3] This allows us to consider the evolution of the radical pair spin at $H>A$ assuming that the nuclear spin does not flip. It means that the analysis carried out in the paper[3] may be applied separately for the two nuclear-spin states $I_z=\pm 1/2$, taking into account that transitions between the radical pair states are enabled by both the external magnetic field and the hyperfine interaction. The corresponding matrix elements read[1]

$$\langle S,I_z|\mathcal{H}|T_0,I_z\rangle=\frac{1}{2}\Delta g\mu_B H\pm\frac{1}{4}\mu_B A$$

with signs plus and minus corresponding to two possible projections of the nuclear spin $I_z=\pm 1/2$ onto the direction of the magnetic field; $\Delta g=g_1-g_2$.

The evolution of a radical pair is described by the density matrix $\rho^{\pm}_{\alpha\beta}(t)$ where Greek indices take the values S, T_0, and $T_{\pm}$. Only diagonal elements of the matrix with respect to the nuclear-spin projections I_z are kept. Collisions of kinks with obstacles result in uncorrelated radical pairs which occupy all eight available spin states with equal probability. Therefore, the initial values of the diagonal elements of the corresponding density matrix are

$$\rho^{\pm}_{SS}(0)=\rho^{\pm}_{T_0T_0}(0)=\frac{1}{8}. \tag{2}$$

Off-diagonal matrix elements with respect to the electron-spin projections are assumed to be zero.

The important parameter of our model determining plastic properties of crystals in magnetic field is the probability $\rho_{SS}(H)$ of occupation of the strongly binding S states. The quantity

$$\rho_{SS}(H)=\rho^{+}_{SS}(H)+\rho^{-}_{SS}(H) \tag{3}$$

can be obtained by solving equations for the density matrix with the Hamiltonian (1) and with the initial conditions (2). This solution is similar to that described in our paper.[3] Then the S-state occupation probabilities with different values of the nuclear-spin projections are

$$\rho^{\pm}_{SS}(H)=\frac{1}{8}\,\frac{(1+T_1/\tau_0)(1+T_2/\tau_0)+(H\pm H_A)^2/H_m^2}{(1+T_1/\tau_0)(1+T_2/\tau_0)+(1+\tau_0/2T_1)(H\pm H_A)^2/H_m^2}. \tag{4}$$

Here

$$H_A=\frac{A}{2\Delta g},\quad H_m=\frac{\hbar}{\Delta g\mu_B\sqrt{T_1T_2}}.$$

The longitudinal spin-relaxation time T_1 is the time of the spin-lattice relaxation of the short-lived T_0 state; T_2 is the transversal spin relaxation time; τ_0 is the average time during which a radical kink-obstacle pair passes the region where a resonance between its S and T_0 states takes place. The magnetic field H_m characterizing the intercombination transitions is at low temperatures of the order of tens of kOe.[3] The field H_A characterizes the range of the magnetic fields where the hyperfine interaction plays an important role. At typical values of the parameters $\Delta g\approx 10^{-3}$ and A ranging from 1 to 100 Oe this field may vary in a broad interval between 0.5 and 50 kOe.

A change of the mechanism responsible for the spin evolution occurs at a magnetic field close to H_A. At $H<H_A$ the principal part in the evolution dynamics is played by the hyperfine interaction, whereas at higher magnetic fields $H>H_A$ this role is taken over by the Δg mechanism. The introduction of the hyperfine interaction results in a qualitative change of the magnetic-field dependence of the plastic properties of crystals. According to our model this dependence is controlled by the function $\rho_{SS}(H)$ which depends on H very weakly in the range $H<H_A$. A stronger dependence starts only at $H>H_A$. Accordingly, one expects a threshold-type behavior near the field H_A in magnetic-field dependences of various plasticity-related phenomena.

Since all elements in the Periodic Table have magnetic isotopes,[10] one should expect that such a threshold will be the rule rather than an exception. Such a threshold was revealed recently with $H_A\approx 2$ kOe in the measurements[11] of the magnetic-field dependence of the external stress-induced dislocation ranges in Al, NaCl, and LiF. It is worth mentioning also that similar thresholds have been often observed in chemical reactions in a magnetic field[1,2,12] where a similar theoretical interpretation has been applied successfully.

Now the role of the hyperfine interaction in the magnetic-field dependence of the amplitude-independent internal friction is discussed. Corresponding measurements in Cu were reported in Ref. 13 and a theory was developed in Ref. 4. It has been demonstrated that the magnetic-field correction to the internal friction of dislocations Q^{-1} shows up at low temperatures due to two mechanisms: an increase of the electron component of the viscous drag of dislocations, and an increase of the probability of depinning from paramagnetic obstacles. The theory agrees well, especially for deformed samples, with the experimental data in the range $1.7\leqslant H\leqslant 12$ kOe where the measurements[13] have been carried out.

The model[4] is applied to determine the influence of the hyperfine interaction on internal friction (measured by applying oscillating shear deformations). Considering preliminary deformed samples, the role of the Kravchenko mechanism[8] is strongly suppressed and the dependence of Q^{-1} on H is determined mainly by the variation of the average dislocation free segment length L_c which according to Ref. 3 reads

$$L_c(H)=L_c(0)\,\frac{\rho_{SS}(0)}{\rho_{SS}(H)}, \tag{5}$$

where Eqs. (3) and (4) should be used to account for the hyperfine interaction. The exact value of the parameter H_A is

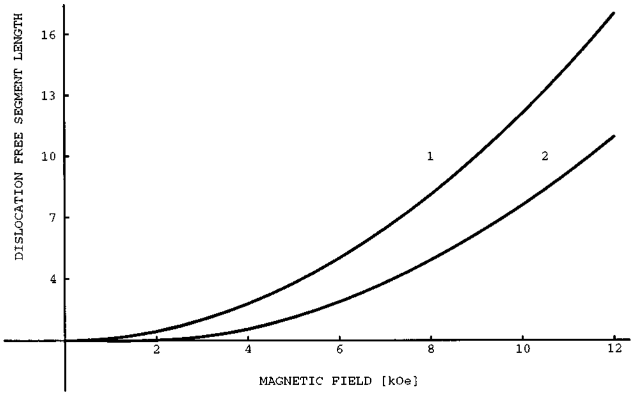

FIG. 1. Average free segment length of dislocation [in units of $L_c(0)$] versus magnetic field without (curve 1) and with (curve 2) account of the hyperfine interaction. The dashed line shows the value $L_c(0)$.

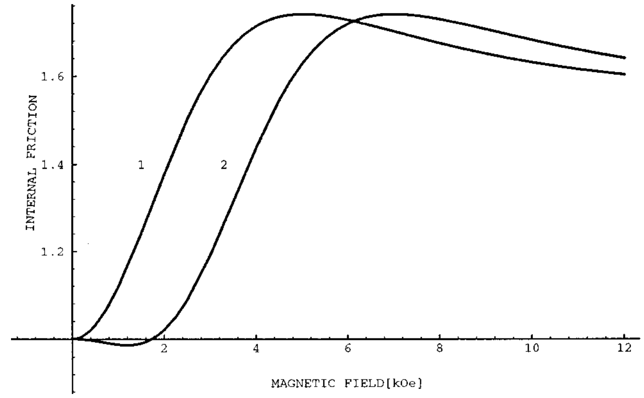

FIG. 2. Amplitude-independent internal friction of dislocations [in units of $Q^{-1}(0)$] versus magnetic field without (curve 1) and with (curve 2) account of the hyperfine interaction.

not known for Cu, so the value $H_A = 2$ kOe as in the experiments[11] is chosen for rough estimates. We also assume that $H_m = 30$ kOe and $\tau_0/T_1 = \tau_0/T_2 = 200$.[3] The other parameters are taken from Ref. 4.

Figure 1 shows that the hyperfine interaction results in a threshold in the dependence $L_c(H)$ near the field H_A. At lower fields the correction to the free segment length $L_c(H)$ decreases slightly whereas at higher field it grows rapidly with the field.

Using the dependence (5) in the model outlined in Ref. 4 the magnetic-field dependence of the internal friction of dislocations is found. Figure 2 demonstrates that the hyperfine interaction changes drastically the behavior of the internal friction at low magnetic fields $H < H_A \approx 2$ kOe where experimental data are still not available. One observes a threshold-like behavior near H_A after which the amplitude-independent internal friction grows with the field. Even stronger dependence and a sharper threshold are expected in the amplitude-dependent internal friction whose decrement depends exponentially on the length L_c.[14]

Revealing these predicted thresholds in internal friction phenomena will be crucial for testing the proposed ideas on the fundamental role of the hyperfine interaction in the formation of plastic properties of crystals in a weak magnetic field. The role played by the dislocation depinning from magnetic obstacles in a magnetic field was earlier discussed for the magnetoplastic[5] and electroplastic[6] effects and for the work hardening[7] in the magnetic field. The results of this paper allow one to introduce the hyperfine interaction in those calculations as well. Then one can expect an observation of various isotope effects in plasticity-related phenomena, since by changing the isotope content one can change characteristics of the hyperfine interaction (such as the magnetic field H_A) and, hence, change magnetic dependences of the measured quantities. For example, replacing magnetic nuclei by their spinless isotopes would lower the threshold, or even remove it completely.

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